

**Appl. No.** : **09/919,739**  
**Filed** : **July 31, 2001**

### **REMARKS**

The preamble of Claim 3 has been amended to clarify that the constructed model is useful for predicting whether a test molecule has a chemical or biological property of interest. Support for this amendment may be found in the specification, for example, at page 4, lines 25-28 and page 10, lines 8-11. Claim 3 has also been amended to recite that whether the reference molecules in the training set have the property of interest is based on experimental data. Support for this amendment may be found in the specification, for example, at page 14, lines 5-8.

Claims 3, 6-8, and 19 remain pending in the application. The Applicants have carefully considered all of the Examiner's rejections but respectfully submit that the claims are allowable for at least the following reasons.

#### Rejections under § 112 – Enablement

The Examiner rejected Claims 3, 6-8, and 19 under 35 U.S.C. § 112, ¶ 1 as being not enabled. The Examiner asserted that the specification was enabling for a molecule T to predict the molecular behavior of high protein binding but not for any chemical or biological property. The Examiner specifically argued that a given biological or chemical property is not necessarily a predictor of molecular behavior.

The claims are directed to the construction of predictive models in which molecules that are experimentally known to have a particular chemical property are used to identify other molecules that possess the same chemical property without needing to perform any physical experiments on the other molecules. This can be illustrated using solubility as an example chemical property. The claims are directed to creating models that use known and experimentally tested soluble molecules to predict whether or not another molecule will be soluble without actually performing a physical solubility experiment on the other molecule. The claims are not directed to creating models that would use solubility to predict another different chemical behavior such as toxicity, affinity to a protein, etc. In the terms used in Claim 3, the “chemical property” exhibited by molecule T is the same as the chemical property being predicted by a model having molecule T as a marker molecule. Because of the identity between the chemical property being used as a predictive starting point and the chemical property being

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predicted at the end, the enablement problem set forth by the Examiner that “a biological or chemical property is not necessarily a predictor of molecular behavior” is not present. Solubility is predictive of solubility, binding is predictive of binding, etc. The Examiner’s reasoning is based on the possibility that the “chemical property” and the “molecular behavior” set forth in Claim 3 are different. In the present invention (and Claim 3 has been amended above to clarify this), solubility is used to predict solubility, binding is used to predict binding, etc. When the starting point and ending prediction are the same, the predictive value of the molecule T of the claim is fully enabled throughout the genus of chemical properties by the specification as filed.

To clarify this point in the claim language, the Applicants have amended Claim 3 to recite that it is directed to constructing a model for predicting whether “a test molecule has a chemical or biological property of interest.” Reference molecules used in the training set are all identified as either possessing or not possessing “said chemical or biological property of interest...based on experimental data.” Claim 3 has therefore been amended to clearly require identity between the chemical or biological property of interest possessed by molecule T (known by experiment) and the chemical or biological property predictions produced by the model that uses molecule T as a marker molecule.

Accordingly, the claimed method is not directed to predicting molecular behavior in general but rather to predicting one or more specific chemical or biological properties of interest by defining marker molecules that have been tested experimentally for the specific chemical or biological property of interest. The claimed method will not require undue experimentation in order to select marker molecules that can be used to predict the presence of that chemical or biological property of interest in a test molecule. As such, the Applicants respectfully submit that the claims are enabled.

### CONCLUSION

The Applicants respectfully submit that the amendments to Claim 3 require only a cursory review by the Examiner and that it is therefore appropriate for the Examiner to enter them. By the foregoing amendments and arguments, the Applicants respectfully submit that they have overcome the Examiner’s rejections and request a timely issuance of a Notice of Allowance.

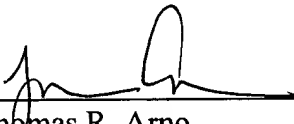
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Please charge any additional fees, including any fees for additional extension of time, or credit overpayment to Deposit Account No. 11-1410.

Respectfully submitted,

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